

# Resonance tunneling of polaritons in 1-D chain with a single defect

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## Abstract

We consider propagation of coupled waves (polaritons) formed by a scalar electromagnetic wave and excitations of a finite one dimensional chain of dipoles. It is shown that a microscopic defect (an impurity dipole) embedded in the chain causes resonance tunneling of the electromagnetic wave with the frequency within the forbidden band between two polariton branches. We demonstrate that resonance tunneling occurs due to local polariton states caused by the defect.

Recently, there has been increasing interest in a novel kind of local states that occur with frequencies inside a gap between different polariton branches (“restrahlen” region) when a dipole active defect is embedded in a regular ionic crystal. These states are coupled states of transverse electromagnetic waves and excitations of a crystal such as phonons or excitons with both components localized in the vicinity of the defect. Rupasov and Singh [1] considered states of a two-level atom coupled with elementary excitations of a medium. A two-level atom considered in that paper could be called an “active” defect since it introduces new modes (transitions between levels of the atom), which were absent in the pure system. The local states associated with such a defect are the original states of an atom modified by the interaction with its surroundings. Correspondingly the frequency of the arising local state is the initial frequency of an internal mode of the defect renormalized by the interaction with the medium.

In our recent papers [2,3] we considered a qualitatively different situation. We showed that a defect ion with no internal degrees of freedom embedded in a regular ionic crystal can give rise to local polariton states. This kind of defects can be called a “passive” defect, and local states predicted in Refs. [2,3] occur due to fundamental reconstruction of the spectrum of a pure system. As a result of such a reconstruction, a discrete eigenfrequency splits from the continuous spectrum giving rise to a local state.

This phenomenon is well known in systems of phonons or excitons and was originally discovered by Lifshitz [4] (see also Refs. [5,6]). Similar effects were also found for electromagnetic waves in photonic crystals [7–9] due to macroscopic defects embedded in their structure. Despite all the differences between local phonon states and local photon states in photonic crystals, they share many common features. For example, local states in both systems could appear in a 3-D system only if the difference between the defect parameters (like a mass or an elastic constant) and corresponding parameters of elements forming the pure structure exceeds a certain threshold. The local polariton states are essentially different from the states considered in Ref. [1] as well as from local phonon states and from photon states in photonic crystals. The most important general result obtained in Refs. [2,3] is that a microscopic passive defect is able to rebuild the spectrum of electromagnetic excitations in the medium in the region of wavelengths much greater than the size of the defect. Another striking difference between these local polaritons and other kinds of local states arising due to passive defects is the absence of a threshold for such states in isotropic systems even in 3-D situation. (For obvious reasons there is no threshold for local states due to “active” defects in any dimensions.)

In the present paper, we show that a dipole-active defect without additional degrees of freedom embedded in an otherwise ideal structure causes resonance tunneling of electromagnetic waves through the forbidden band. A similar effect have been observed in a thin slab of a photonic crystal with a defect [7]. We would like to emphasize, however, that we discuss resonance tunneling of electromagnetic waves with wavelengths much greater than the characteristic scale of the defect, while in the case of photonic crystals one deals with the situation when the wavelength is comparable with the size of a macroscopic distortion of the periodicity. We show that the resonance transmission in the stop-band occurs due to local polariton states associated with the defect. Experimental observation of this effect seems very promising and could be an unambiguous indication for local polaritons.

Another question that we would like to address is related to the fact that local polaritons

arise as a superposition of polariton modes from the entire Brillouin band. Excitations with wave numbers at the edge of the band are pure phonons and electromagnetic waves. In order to make sure that short-wavelength components of the electromagnetic field do not destroy the effect one must consider a model feasible for the microscopic treatment of the field. In order to shed light on principle aspects of the problems outlined above, we study light propagation through a one-dimensional finite chain of dipoles with the nearest neighbor interaction. We assume that this chain is placed within a single mode waveguide. Polaritons in this system arise as coupled states of collective excitations of dipoles (polarization waves) and electromagnetic waves. An important feature of the model is accounting for the interaction between dipoles at different sites that leads to spatial dispersion of the polarization waves. Taking into account the spatial dispersion makes the exact analytical consideration of the problem unfeasible even in the case of a pure system due to cumbersome algebra. Therefore, we carry out numerical simulations by means of the transfer-matrix method. The model can be described by the following equations written in the frequency domain:

$$(\Omega_n^2 - \omega^2)P_n + \Phi(P_{n+1} + P_{n-1}) = \alpha E(x_n), \quad (1)$$

$$\frac{\omega^2}{c^2}E(x) + \frac{d^2 E}{dx^2} = -4\pi \frac{\omega^2}{c^2} \sum_n P_n \delta(na - x), \quad (2)$$

where the first equation describes the dynamics of site dipole moments,  $P_n$ , and the second one is the equation for the electric field  $E$ . Here  $\Omega_n$  is the diagonal part of the force matrix responsible for the short-range interaction between dipoles, and  $\Phi$  is its off-diagonal component. We assume that the defect, which occupies the site  $n_0$  affects only the diagonal part of the force matrix, so that  $\Omega_n = \Omega$  for all  $n$  except for  $n = n_0$ , where  $\Omega_{n_0} = \Omega_{def}$ . The coordinate  $x$  in Eq. (2) goes along the chain with the interatomic distance  $a$ , and the right hand side of this equation is the microscopic polarization density. Parameter  $\alpha$  is responsible for coupling between polarization and electromagnetic waves. Eqs. (1, 2) present *microscopic* description of the transverse electromagnetic waves propagating along the chain. These equations are subject to the boundary conditions for the electromagnetic and polarization subsystems. We assume that an incident and transmitted electromagnetic waves propagate in vacuum so that the boundary conditions for Eq. (2) take the usual form

$$E(0) = 1 + r; \quad \frac{dE}{dx} = ik(1 - r); \quad (3)$$

$$E(L) = t \exp(ikL); \quad \frac{dE}{dx} = ikt \exp(ikL), \quad (4)$$

where  $k = \omega/c$  is a wave number of the electromagnetic wave in vacuum,  $|t|^2$  and  $|r|^2$  are transmission and reflection coefficients, respectively, and  $L$  is the length of the chain. The boundary conditions for dipole excitations can be chosen in the general form

$$\frac{P_0}{P_1} = \beta; \quad \frac{P_N}{P_N - 1} = \gamma, \quad (5)$$

where  $N = L/a$  is the number of sites in the chain, parameters  $\beta$  and  $\gamma$  describe different states of the “surface” of the chain. For example,  $\beta = 0$ ,  $\gamma = 0$  correspond to the chain with

fixed terminal points. Another set of parameters,  $\beta = 1$ ,  $\gamma = 1$ , describes a “relaxed surface” where the forces on terminal sites are equal to zero. We present results of calculations with these two choices of the boundary conditions.

Our first goal is to convert the differential equation (2) into the discrete form. We can do this considering separately free propagation of electromagnetic waves between sites and its scattering due to the interaction with a dipole moment at the site. Let  $E_n$  and  $E'_n$  be the magnitude of the electromagnetic field and its derivative right after scattering at the  $n$ th site. The electric field  $E$  remains continuous at a scattering site, while its derivative undergoes the jump, which is equal to  $-4\pi k^2 P_n$ . Finally, one can derive the system of difference equations, that can be written with the use of the transfer matrix,  $T$ , in the form:

$$v_{n+1} = T_n v_n, \quad (6)$$

where we introduced the column vector,  $v_n$ , with components  $P_n$ ,  $P_{n+1}$ ,  $E_n$ ,  $D_n$  ( $D_n = E'_n/k$ ) and the transfer matrix,  $T_n$ , that describes the propagation of the vector between adjacent sites:

$$T_n = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & -\frac{\Omega_n^2 - \omega^2}{\Phi} & \frac{\alpha}{4\pi} \cos ka & \frac{\alpha}{4\pi} \sin ka \\ 0 & 0 & \cos ka & \sin ka \\ 0 & -4\pi k & -\sin ka & \cos ka \end{pmatrix}. \quad (7)$$

The dynamical state of the system at the right end of the chain, which is represented by the vector  $v_N$ , can be found from the initial state at the left end,  $v_0$ , by means of the repetitive use of the transfer matrix,  $T$  :

$$v_N = \prod_1^N T_n v_0. \quad (8)$$

Since we consider the system with a single defect, all but one  $T$ -matrices in Eq. (8) are the same. These matrices have the parameter  $\Omega_n$  (the only parameter, which distinguish the defect site from the regular sites) equal to  $\Omega$ . For the matrix  $T_{n_0}$ , which corresponds to the defect,  $\Omega_n = \Omega_{def}$ . The eigenfrequencies of the pure system, i.e. polariton dispersion laws, can be found by means of the eigenvalues of the  $T$ -matrix. There exist four eigenvalues  $\lambda$ , which can be grouped in pairs with the product of the members of each pair being equal to one. The eigenvalues can be found as solutions of the following dispersion equation:

$$\left( \lambda + \lambda^{-1} - 2 \cos ka \right) \left( \lambda + \lambda^{-1} + \frac{\Omega^2 - \omega^2}{\Phi} \right) + 4\pi k \sin(ka) = 0. \quad (9)$$

In the band of propagating states, the solutions of Eq. (9) are complex valued numbers with their absolute values equal to one. In this case the expression  $\lambda + \lambda^{-1}$  can be presented in the form:  $2 \cos(Qa)$ , where  $Q$  is the Bloch wave number. With this replacement the dispersion equation (9) takes the same form as the equation obtained from the original Eqs. (1, 2) by means of Fourier transformation. It is important to emphasize that Eq. (9) takes into account the modes of the electromagnetic field not only from the first Brillouin band but also all short-wave components of the field. In this sense, our approach to the problem is

truly microscopic. In the band gap of the polariton spectrum, the eigenvalues  $\lambda$  become real valued and describe evanescent modes of the system. Fig.1 presents the frequency dependence of the absolute value of one of the eigenvalues. The band gap is clearly seen as a region in which the absolute value of  $\lambda$  is greater than 1.

We calculated the transmission coefficient of the electromagnetic waves applying Eq. (8) to the vector  $v_0$ , with components  $\{P_0, \beta P_0, 1 + r, i(1 - r)\}$ , which describes the state of electromagnetic waves and dipole subsystem at the left end of the chain in accordance with boundary conditions (3) and (5). The resulting state at the right end of the chain  $v_N$  is to be matched with the corresponding boundary conditions at  $n = N$ . We considered two kinds of boundary conditions corresponding to fixed,  $\beta = \gamma = 0$ , and relaxed,  $\beta = \gamma = 1$ , ends of the chain. For the numeric evaluation we use the chain consisting of 30 atoms, with the defect placed at the 5th site. In order to check the computations, we calculated both transmission and reflection coefficients and verified that the equality  $|t|^2 + |r|^2 = 1$  holds with sufficient accuracy.

The results of the calculations are presented in Figs.2 and 3, which correspond to the fixed and relaxed boundary conditions respectively. The parameter of the nearest neighbors interaction  $\Phi$  was chosen to be equal to  $\Phi = \Omega^2/3$ , so that the maximum frequency of the polarization waves is equal to  $\sqrt{5/3}\Omega$ . As one can see from Fig.1, the polariton gap has a lower boundary at a slightly lower frequency,  $\simeq 1.24\Omega$ . It is caused by the negative dispersion of the polariton waves assumed in the calculations. The frequency in all the figures is normalized by  $\Omega$ . The wavelength of the electromagnetic waves in the region considered is much greater than the interatomic distance  $a$ , the product  $ka$  is of order of  $10^{-3}$ , which corresponds to the position of the exciton-polariton gap in real materials. Figs.2a and 3a present the frequency dependence of the transmission in the pure system for two types of boundary conditions. One can easily recognize the boundary between the pass and stop bands in these figures. The transmission exhibits a rich structure, corresponding to geometrical resonances due to the finite size of the system in the pass band, and monotonically increases with the frequency in the forbidden band. The increase of the transmission is due to the frequency dependence of the penetration length  $l = 1/\text{Im } q(\omega)$ , where  $q(\omega)$  is the imaginary wave number of polaritons inside the gap.

All the other plots in Figs.2 and 3 show the transmission in a system containing the defect for different values of the parameter  $\Delta = (\Omega_{def}^2 - \Omega^2)/\Omega^2$ , which determines the strength of the defect. One can see that the defect induces a resonant maximum at a certain value of frequency,  $\omega_r$ , inside the forbidden gap. Though resonance tunneling takes place for both kinds of boundary conditions, the effect is much more prominent in the case of fixed ends. This fact is in agreement with the overall greater transmission for the latter situation than in the case of “relaxed” ends. The positions of the maxima was found to be independent of the position of the defect in the chain as it should be expected. We set the defect at different sites and found just a slight modification of the shape of the maxima and their heights, but not the positions.

The value of  $\omega_r$  depends upon the strength of the defect, it moves toward higher frequencies with increase of  $\Delta$ . This behavior is in accord with the results of Refs. [2,3] regarding the eigenfrequencies of local polariton states. For the model considered the frequency of the local polariton is determined by an equation similar to that obtained in Ref. [2],

$$1 = \Delta \int_{-\pi}^{\pi} \frac{\cos(ka) - \cos x}{\left(k^2 - 1 - \frac{2\Phi}{\Omega^2} \cos x\right) (\cos(ka) - \cos x) - \frac{\alpha k}{2} \sin(ak)} dx \quad (10)$$

In Fig. 4 we present the dependence of the resonance frequency,  $\omega_r$ , and the eigenfrequency of the local mode upon the defect parameter,  $\Delta$ . One can see that these dependences are consistent with each other. The deviation of  $\omega_r$  from the eigenfrequency is obviously due to the frequency dependence of the width of the resonance.

According to Eq. (10), local polaritons arise only for positive  $\Delta$ . Indeed, when we change the sign, the resonance maximum inside the stop-band disappears (Fig. 5). At the same time, one can identify in Fig. 5a a new peak in the pass band, which arises due to the defect. Though there are no new eigenstates in the region of the continuous spectrum, the defect, nevertheless, causes resonance scattering of propagating polaritons. This effect is known as quasilocal or resonance “states,” for example, in phonon physics [5,6], and was discussed for polaritons by Hopfield [10]. The defect-induced maximum observed in the pass band in Fig. 5a is caused by such “quasilocal states.” Surprisingly enough, is the absence of a quasilocal resonance in Fig. 5b. This represents the transmission in the case of “free” surface. Instead, we observe a strong dip in the transmission which was not present in the transmission of the pure chain. This situation of antiresonance scattering is interesting but requires separate consideration.

In conclusion, we have numerically shown that an electromagnetic wave with frequency within the forbidden polariton band (“restrahlen region”) can exhibit resonance tunneling via a microscopic defect, for example, an impurity atom. The tunneling is due to the local polariton states associated with the defect. Electromagnetic waves were treated in the paper microscopically in the sense that we took into account the lattice structure of the medium and all the modes of the electromagnetic field including those with wave lengths shorter than  $\pi/a$ . The results of the calculations showed that the short-wave components of the electromagnetic field indeed do not contribute considerably to the effect, which is in agreement with the assumption of Ref. [2]. The observed effects occurred for long waves with wavelengths three orders of magnitude greater than the interatomic distance.

Though we have considered the one-dimensional single-mode model, the main result obtained in the paper – the existence of resonance tunneling of electromagnetic waves due to the local polariton states – can be expanded to more realistic situations. The one dimensional nature of the model allowed for the microscopic treatment, which would not be feasible otherwise. Once we have confirmed the assumption of Ref. [2] regarding the role of shortwave component of electromagnetic waves, one can treat the system in the framework of macroscopic methods and turn to the consideration of more realistic models. Though the resonance tunneling through a thin slab of a real 3-D material will have more complicated properties, the essence of the effect will remain the same.

The most serious difference between our single-mode model of electromagnetic waves and real situations is the absence of longitudinal modes in our model. These modes could fill the gap between polariton branches and reduce the lifetime of local polaritons. It is important to emphasize, however, that unlike the above mentioned quasilocal states of propagating modes, the transverse components of the local polariton remains localized. Therefore the tunneling nature of electromagnetic wave propagation through the restrahlen region is preserved even in the presence of the longitudinal modes.

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## CAPTIONS

Fig. 1. Frequency dependence of the absolute value of an eigenvalue of the transfer matrix  $T$ . In the pass band, the absolute value of  $\lambda$  is equal to 1, in the stop band it is greater than 1.

Fig. 2. Transmission through the chain with fixed ends. (a) corresponds to the pure system, (b) and (c) describes the transmission through the system with the defect for the different strength  $\Delta$ .

Fig. 3. Same as in Fig. 2 but for the chain with free ends.

Fig. 4. The solid line represents the relationship between eigenfrequencies of the local polaritons and the defect parameter  $\Delta$ . Two dashed lines show the positions of the resonance tunneling maxima for different  $\Delta$ . The upper dashed line corresponds to the chain with fixed ends, and the lower one presents the results for the chain with free ends.

Fig. 5. Quasilocals states in the pass band for the chain with (a) fixed and (b) free ends.

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truly microscopic. In the band gap of the polariton spectrum, the eigenvalues  $\lambda$  become real valued and describe evanescent modes of the system. Fig.1 presents the frequency dependence of the absolute value of one of the eigenvalues. The band gap is clearly seen as a region in which the absolute value of  $\lambda$  is greater than 1.

We calculated the transmission coefficient of the electromagnetic waves applying Eq. (8) to the vector  $v_0$ , with components  $\{P_0, \beta P_0, 1 + r, i(1 - r)\}$ , which describes the state of electromagnetic waves and dipole subsystem at the left end of the chain in accordance with boundary conditions (3) and (5). The resulting state at the right end of the chain  $v_N$  is to be matched with the corresponding boundary conditions at  $n = N$ . We considered two kinds of boundary conditions corresponding to fixed,  $\beta = \gamma = 0$ , and relaxed,  $\beta = \gamma = 1$ , ends of the chain. For the numeric evaluation we use the chain consisting of 30 atoms, with the defect placed at the 5th site. In order to check the computations, we calculated both transmission and reflection coefficients and verified that the equality  $|t|^2 + |r|^2 = 1$  holds with sufficient accuracy.

The results of the calculations are presented in Figs.2 and 3, which correspond to the fixed and relaxed boundary conditions respectively. The parameter of the nearest neighbors interaction  $\Phi$  was chosen to be equal to  $\Phi = \Omega^2/3$ , so that the maximum frequency of the polarization waves is equal to  $\sqrt{5/3}\Omega$ . As one can see from Fig.1, the polariton gap has a lower boundary at a slightly lower frequency,  $\simeq 1.24\Omega$ . It is caused by the negative dispersion of the polariton waves assumed in the calculations. The frequency in all the figures is normalized by  $\Omega$ . The wavelength of the electromagnetic waves in the region considered is much greater than the interatomic distance  $a$ , the product  $ka$  is of order of  $10^{-3}$ , which corresponds to the position of the exciton-polariton gap in real materials. Figs.2a and 3a present the frequency dependence of the transmission in the pure system for two types of boundary conditions. One can easily recognize the boundary between the pass and stop bands in these figures. The transmission exhibits a rich structure, corresponding to geometrical resonances due to the finite size of the system in the pass band, and monotonically increases with the frequency in the forbidden band. The increase of the transmission is due to the frequency dependence of the penetration length  $l = 1/\text{Im } q(\omega)$ , where  $q(\omega)$  is the imaginary wave number of polaritons inside the gap.

All the other plots in Figs.2 and 3 show the transmission in a system containing the defect for different values of the parameter  $\Delta = (\Omega_{def}^2 - \Omega^2)/\Omega^2$ , which determines the strength of the defect. One can see that the defect induces a resonant maximum at a certain value of frequency,  $\omega_r$ , inside the forbidden gap. Though resonance tunneling takes place for both kinds of boundary conditions, the effect is much more prominent in the case of fixed ends. This fact is in agreement with the overall greater transmission for the latter situation than in the case of “relaxed” ends. The positions of the maxima was found to be independent of the position of the defect in the chain as it should be expected. We set the defect at different sites and found just a slight modification of the shape of the maxima and their heights, but not the positions.

The value of  $\omega_r$  depends upon the strength of the defect, it moves toward higher frequencies with increase of  $\Delta$ . This behavior is in accord with the results of Refs. [2,3] regarding the eigenfrequencies of local polariton states. For the model considered the frequency of the local polariton is determined by an equation similar to that obtained in Ref. [2],

$$1 = \Delta \int_{-\pi}^{\pi} \frac{\cos(ka) - \cos x}{\left(k^2 - 1 - \frac{2\Phi}{\Omega^2} \cos x\right) (\cos(ka) - \cos x) - \frac{\alpha k}{2} \sin(ak)} dx \quad (10)$$

In Fig. 4 we present the dependence of the resonance frequency,  $\omega_r$ , and the eigenfrequency of the local mode upon the defect parameter,  $\Delta$ . One can see that these dependences are consistent with each other. The deviation of  $\omega_r$  from the eigenfrequency is obviously due to the frequency dependence of the width of the resonance.

According to Eq. (10), local polaritons arise only for positive  $\Delta$ . Indeed, when we change the sign, the resonance maximum inside the stop-band disappears (Fig. 5). At the same time, one can identify in Fig. 5a a new peak in the pass band, which arises due to the defect. Though there are no new eigenstates in the region of the continuous spectrum, the defect, nevertheless, causes resonance scattering of propagating polaritons. This effect is known as quasilocal or resonance “states,” for example, in phonon physics [5,6], and was discussed for polaritons by Hopfield [10]. The defect-induced maximum observed in the pass band in Fig. 5a is caused by such “quasilocal states.” Surprisingly enough, is the absence of a quasilocal resonance in Fig. 5b. This represents the transmission in the case of “free” surface. Instead, we observe a strong dip in the transmission which was not present in the transmission of the pure chain. This situation of antiresonance scattering is interesting but requires separate consideration.

In conclusion, we have numerically shown that an electromagnetic wave with frequency within the forbidden polariton band (“restrahlen region”) can exhibit resonance tunneling via a microscopic defect, for example, an impurity atom. The tunneling is due to the local polariton states associated with the defect. Electromagnetic waves were treated in the paper microscopically in the sense that we took into account the lattice structure of the medium and all the modes of the electromagnetic field including those with wave lengths shorter than  $\pi/a$ . The results of the calculations showed that the short-wave components of the electromagnetic field indeed do not contribute considerably to the effect, which is in agreement with the assumption of Ref. [2]. The observed effects occurred for long waves with wavelengths three orders of magnitude greater than the interatomic distance.

Though we have considered the one-dimensional single-mode model, the main result obtained in the paper – the existence of resonance tunneling of electromagnetic waves due to the local polariton states – can be expanded to more realistic situations. The one dimensional nature of the model allowed for the microscopic treatment, which would not be feasible otherwise. Once we have confirmed the assumption of Ref. [2] regarding the role of shortwave component of electromagnetic waves, one can treat the system in the framework of macroscopic methods and turn to the consideration of more realistic models. Though the resonance tunneling through a thin slab of a real 3-D material will have more complicated properties, the essence of the effect will remain the same.

The most serious difference between our single-mode model of electromagnetic waves and real situations is the absence of longitudinal modes in our model. These modes could fill the gap between polariton branches and reduce the lifetime of local polaritons. It is important to emphasize, however, that unlike the above mentioned quasilocal states of propagating modes, the transverse components of the local polariton remains localized. Therefore the tunneling nature of electromagnetic wave propagation through the restrahlen region is preserved even in the presence of the longitudinal modes.

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## CAPTIONS

Fig. 1. Frequency dependence of the absolute value of an eigenvalue of the transfer matrix  $T$ . In the pass band, the absolute value of  $\lambda$  is equal to 1, in the stop band it is greater than 1.

Fig. 2. Transmission through the chain with fixed ends. (a) corresponds to the pure system, (b) and (c) describes the transmission through the system with the defect for the different strength  $\Delta$ .

Fig. 3. Same as in Fig. 2 but for the chain with free ends.

Fig. 4. The solid line represents the relationship between eigenfrequencies of the local polaritons and the defect parameter  $\Delta$ . Two dashed lines show the positions of the resonance tunneling maxima for different  $\Delta$ . The upper dashed line corresponds to the chain with fixed ends, and the lower one presents the results for the chain with free ends.

Fig. 5. Quasilocal states in the pass band for the chain with (a) fixed and (b) free ends.



















